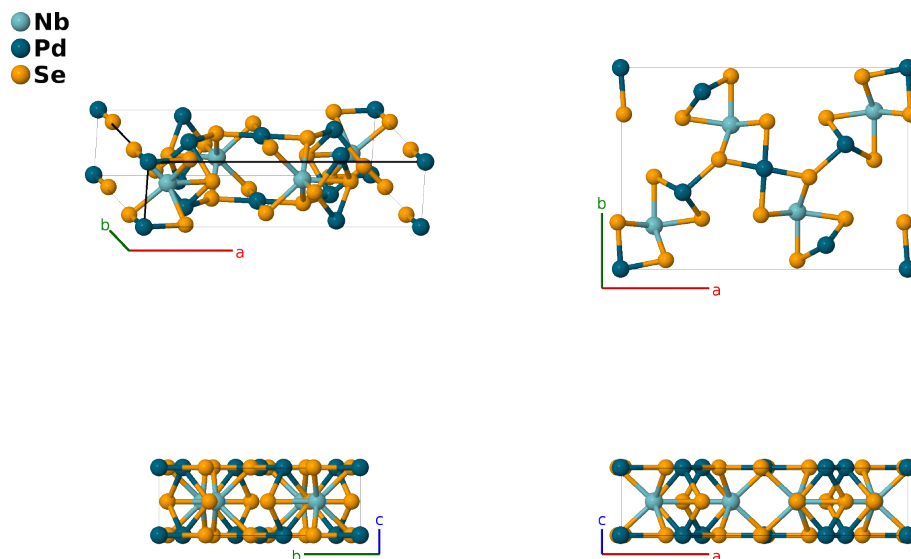# Nb₂Pd₃Se₈ Structure: A2B3C8_oP26_55_h_ag_2g2h-001

This structure originally had the label `A2B3C8_oP26_55_h_ag_2g2h`. Calls to that address will be redirected here.

https://aflow.org/p/X0K9

https://aflow.org/p/A2B3C8_oP26_55_h_ag_2g2h-001

Prototype	$Nb_2Pd_3Se_8$
AFLOW prototype label	A2B3C8_oP26_55_h_ag_2g2h-001
ICSD	49523
Pearson symbol	oP26
Space group number	55
Space group symbol	*Pbam*
AFLOW prototype command	aflow --proto=A2B3C8_oP26_55_h_ag_2g2h-001 --params=$a, b/a, c/a, x_2, y_2, x_3, y_3, x_4, y_4, x_5, y_5, x_6, y_6, x_7, y_7$

Other compounds with this structure

$Ta_2Pd_3Se_8$

Simple Orthorhombic primitive vectors
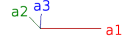
$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
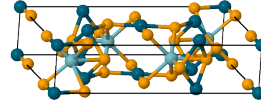$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	0	$=$	0	(2a)	Pd I
$\mathbf{B_2}$	$=$	$\frac{1}{2}\,\mathbf{a_1} + \frac{1}{2}\,\mathbf{a_2}$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(2a)	Pd I
$\mathbf{B_3}$	$=$	$x_2\,\mathbf{a_1} + y_2\,\mathbf{a_2}$	$=$	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}}$	(4g)	Pd II
$\mathbf{B_4}$	$=$	$-x_2\,\mathbf{a_1} - y_2\,\mathbf{a_2}$	$=$	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}}$	(4g)	Pd II
$\mathbf{B_5}$	$=$	$-\left(x_2 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_2 + \frac{1}{2}\right)\mathbf{a_2}$	$=$	$-a\left(x_2 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\hat{\mathbf{y}}$	(4g)	Pd II
$\mathbf{B_6}$	$=$	$\left(x_2 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_2 - \frac{1}{2}\right)\mathbf{a_2}$	$=$	$a\left(x_2 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\hat{\mathbf{y}}$	(4g)	Pd II
$\mathbf{B_7}$	$=$	$x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2}$	$=$	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}}$	(4g)	Se I
$\mathbf{B_8}$	$=$	$-x_3\,\mathbf{a_1} - y_3\,\mathbf{a_2}$	$=$	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}}$	(4g)	Se I
$\mathbf{B_9}$	$=$	$-\left(x_3 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_3 + \frac{1}{2}\right)\mathbf{a_2}$	$=$	$-a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}}$	(4g)	Se I
$\mathbf{B_{10}}$	$=$	$\left(x_3 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_3 - \frac{1}{2}\right)\mathbf{a_2}$	$=$	$a\left(x_3 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}}$	(4g)	Se I
$\mathbf{B_{11}}$	$=$	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2}$	$=$	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}}$	(4g)	Se II
$\mathbf{B_{12}}$	$=$	$-x_4\,\mathbf{a_1} - y_4\,\mathbf{a_2}$	$=$	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}}$	(4g)	Se II
$\mathbf{B_{13}}$	$=$	$-\left(x_4 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_4 + \frac{1}{2}\right)\mathbf{a_2}$	$=$	$-a\left(x_4 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}}$	(4g)	Se II
$\mathbf{B_{14}}$	$=$	$\left(x_4 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_4 - \frac{1}{2}\right)\mathbf{a_2}$	$=$	$a\left(x_4 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}}$	(4g)	Se II
$\mathbf{B_{15}}$	$=$	$x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Nb I
$\mathbf{B_{16}}$	$=$	$-x_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Nb I
$\mathbf{B_{17}}$	$=$	$-\left(x_5 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_5 + \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$-a\left(x_5 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Nb I
$\mathbf{B_{18}}$	$=$	$\left(x_5 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_5 - \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$a\left(x_5 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Nb I
$\mathbf{B_{19}}$	$=$	$x_6\,\mathbf{a_1} + y_6\,\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Se III
$\mathbf{B_{20}}$	$=$	$-x_6\,\mathbf{a_1} - y_6\,\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Se III
$\mathbf{B_{21}}$	$=$	$-\left(x_6 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_6 + \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$-a\left(x_6 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Se III
$\mathbf{B_{22}}$	$=$	$\left(x_6 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_6 - \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$a\left(x_6 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Se III
$\mathbf{B_{23}}$	$=$	$x_7\,\mathbf{a_1} + y_7\,\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Se IV
$\mathbf{B_{24}}$	$=$	$-x_7\,\mathbf{a_1} - y_7\,\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Se IV
$\mathbf{B_{25}}$	$=$	$-\left(x_7 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_7 + \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$-a\left(x_7 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Se IV
$\mathbf{B_{26}}$	$=$	$\left(x_7 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_7 - \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$a\left(x_7 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Se IV

References

[1] D. A. Keszler and J. A. Ibers, *A new structural type in ternary chalcogenide chemistry: Structure and properties of $Nb_2Pd_3Se_8$*, J. Solid State Chem. **52**, 73–79 (1984), doi:10.1016/0022-4596(84)90200-7.